



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2026 – 02:24 PM EDT

PDB ID : 9Q1U / pdb_00009q1u
Title : Borrelia burgdorferi BmpA bound to thymidine
Authors : Liu, Q.; Fernandez, D.; Sharaf, N.G.
Deposited on : 2025-08-14
Resolution : 2.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

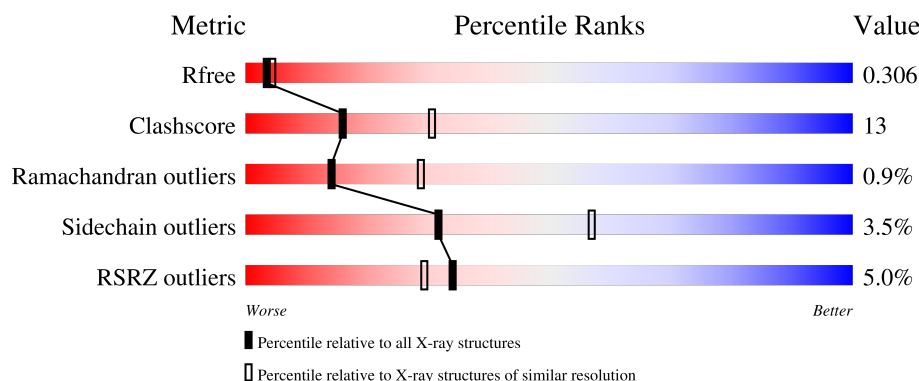
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


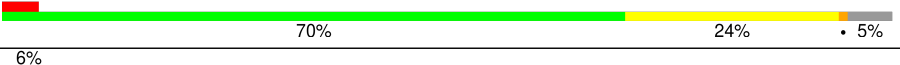
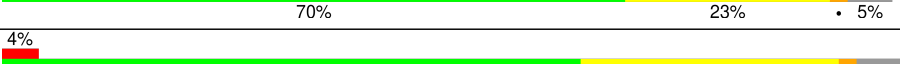
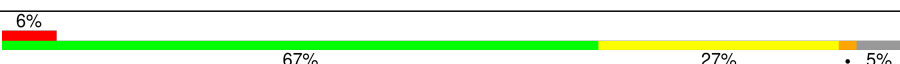

The reported resolution of this entry is 2.58 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	328	
1	B	328	
1	C	328	
1	D	328	
1	E	328	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	328	<div><div></div><div>5%</div><div>62%</div><div>32%</div><div>• 5%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14665 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Basic membrane protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2415	1546	391	474	4			
1	B	313	Total	C	N	O	S	0	0	0
			2415	1546	391	474	4			
1	C	313	Total	C	N	O	S	0	0	0
			2415	1546	391	474	4			
1	D	313	Total	C	N	O	S	0	0	0
			2415	1546	391	474	4			
1	E	313	Total	C	N	O	S	0	0	0
			2415	1546	391	474	4			
1	F	313	Total	C	N	O	S	0	0	0
			2415	1546	391	474	4			

There are 42 discrepancies between the modelled and reference sequences:

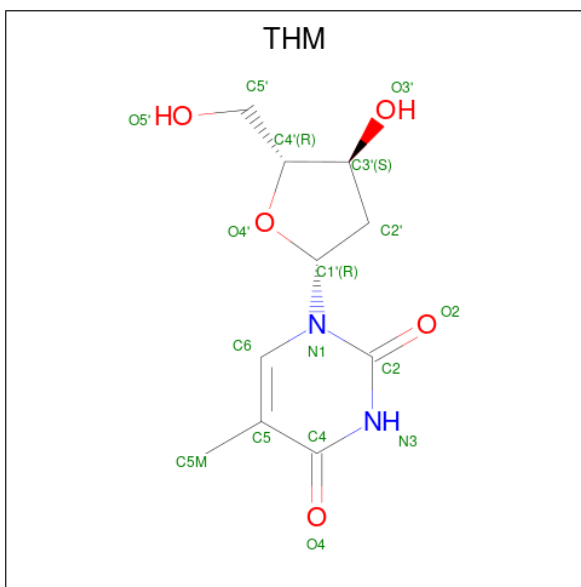
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP Q45010
A	-4	HIS	-	expression tag	UNP Q45010
A	-3	HIS	-	expression tag	UNP Q45010
A	-2	HIS	-	expression tag	UNP Q45010
A	-1	HIS	-	expression tag	UNP Q45010
A	0	HIS	-	expression tag	UNP Q45010
A	1	HIS	-	expression tag	UNP Q45010
B	-5	MET	-	initiating methionine	UNP Q45010
B	-4	HIS	-	expression tag	UNP Q45010
B	-3	HIS	-	expression tag	UNP Q45010
B	-2	HIS	-	expression tag	UNP Q45010
B	-1	HIS	-	expression tag	UNP Q45010
B	0	HIS	-	expression tag	UNP Q45010
B	1	HIS	-	expression tag	UNP Q45010
C	-5	MET	-	initiating methionine	UNP Q45010
C	-4	HIS	-	expression tag	UNP Q45010
C	-3	HIS	-	expression tag	UNP Q45010

Continued on next page...

Continued from previous page...

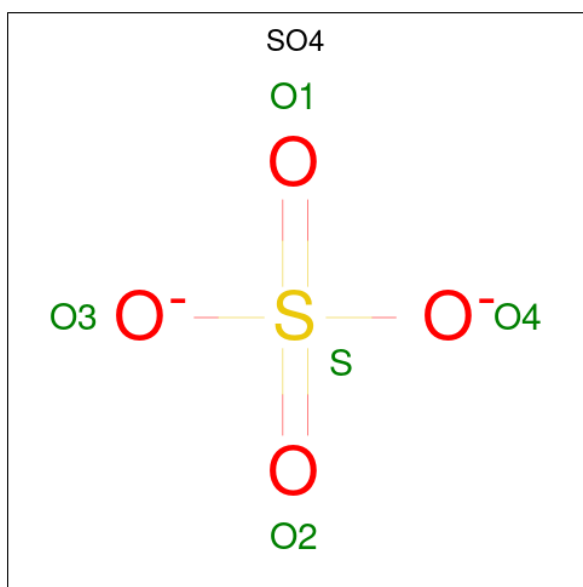
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q45010
C	-1	HIS	-	expression tag	UNP Q45010
C	0	HIS	-	expression tag	UNP Q45010
C	1	HIS	-	expression tag	UNP Q45010
D	-5	MET	-	initiating methionine	UNP Q45010
D	-4	HIS	-	expression tag	UNP Q45010
D	-3	HIS	-	expression tag	UNP Q45010
D	-2	HIS	-	expression tag	UNP Q45010
D	-1	HIS	-	expression tag	UNP Q45010
D	0	HIS	-	expression tag	UNP Q45010
D	1	HIS	-	expression tag	UNP Q45010
E	-5	MET	-	initiating methionine	UNP Q45010
E	-4	HIS	-	expression tag	UNP Q45010
E	-3	HIS	-	expression tag	UNP Q45010
E	-2	HIS	-	expression tag	UNP Q45010
E	-1	HIS	-	expression tag	UNP Q45010
E	0	HIS	-	expression tag	UNP Q45010
E	1	HIS	-	expression tag	UNP Q45010
F	-5	MET	-	initiating methionine	UNP Q45010
F	-4	HIS	-	expression tag	UNP Q45010
F	-3	HIS	-	expression tag	UNP Q45010
F	-2	HIS	-	expression tag	UNP Q45010
F	-1	HIS	-	expression tag	UNP Q45010
F	0	HIS	-	expression tag	UNP Q45010
F	1	HIS	-	expression tag	UNP Q45010

- Molecule 2 is THYMIDINE (CCD ID: THM) (formula: C₁₀H₁₄N₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	10	2	5		
2	B	1	Total	C	N	O	0	0
			17	10	2	5		
2	C	1	Total	C	N	O	0	0
			17	10	2	5		
2	D	1	Total	C	N	O	0	0
			17	10	2	5		
2	E	1	Total	C	N	O	0	0
			17	10	2	5		
2	F	1	Total	C	N	O	0	0
			17	10	2	5		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

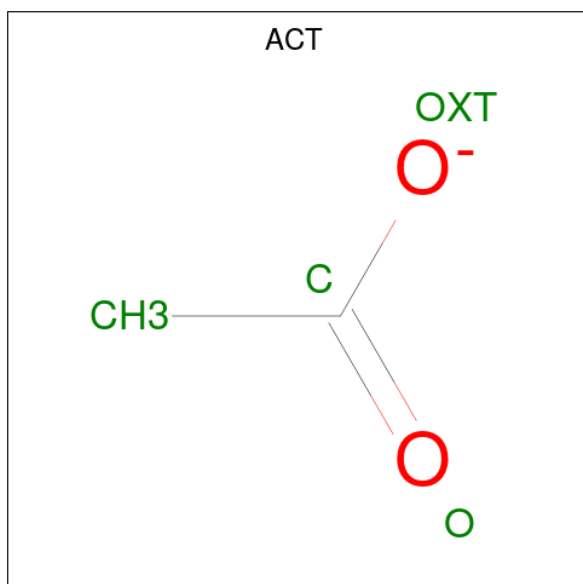


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	C	O	0	0
			4	2	2		

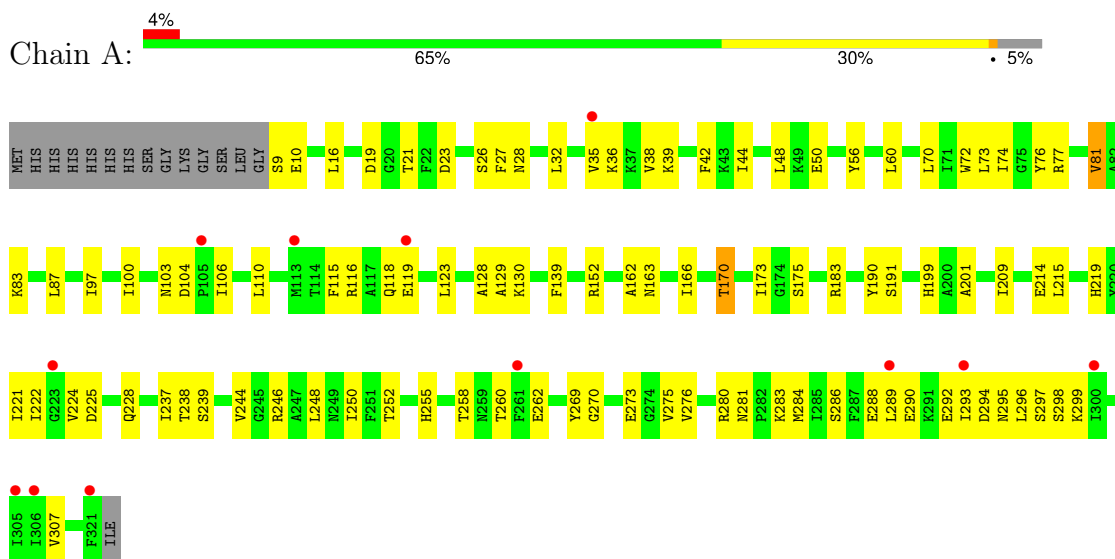
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		
6	B	13	Total	O	0	0
			13	13		
6	C	5	Total	O	0	0
			5	5		
6	D	8	Total	O	0	0
			8	8		
6	E	3	Total	O	0	0
			3	3		
6	F	14	Total	O	0	0
			14	14		

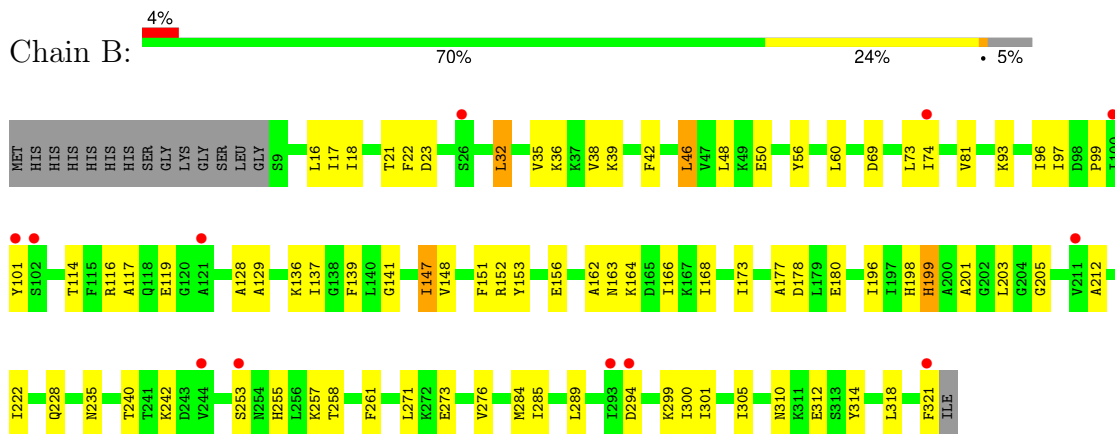
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Basic membrane protein A

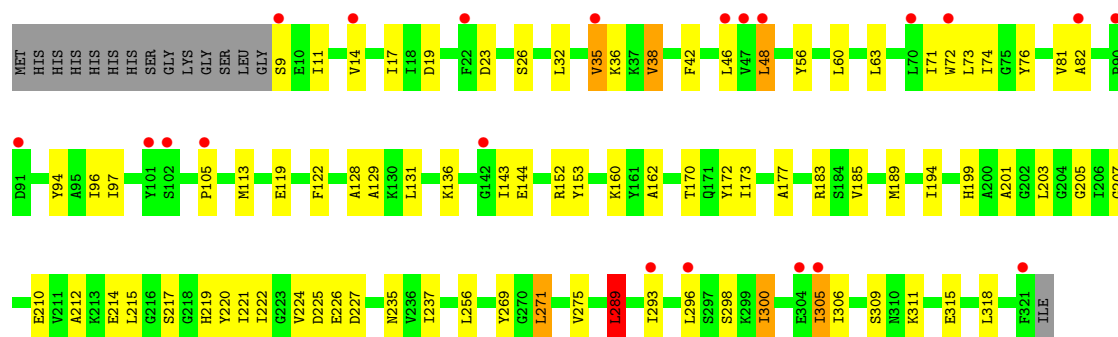


• Molecule 1: Basic membrane protein A

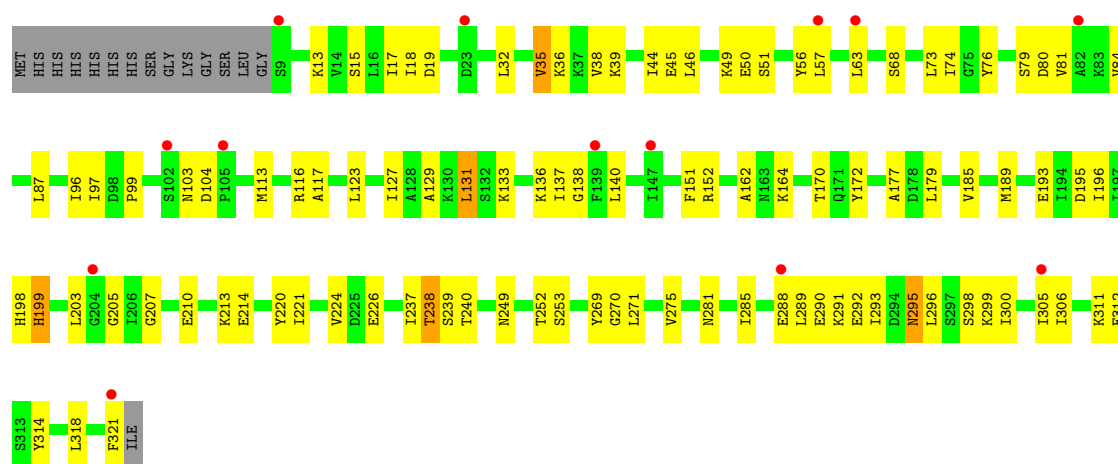


• Molecule 1: Basic membrane protein A

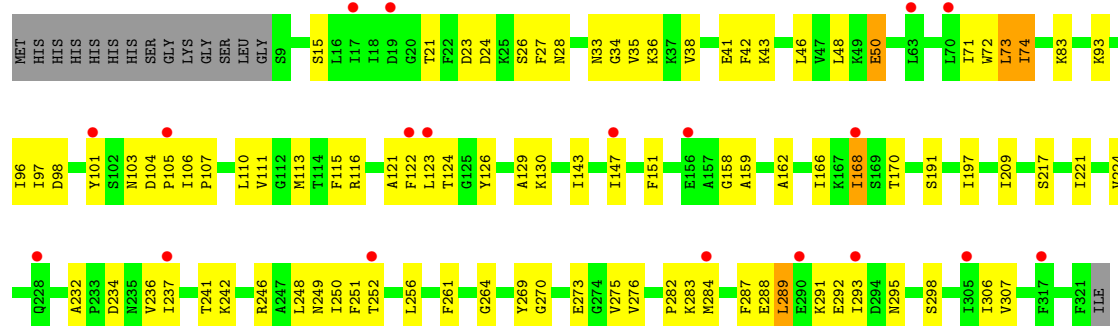




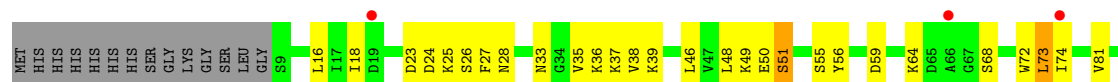
• Molecule 1: Basic membrane protein A

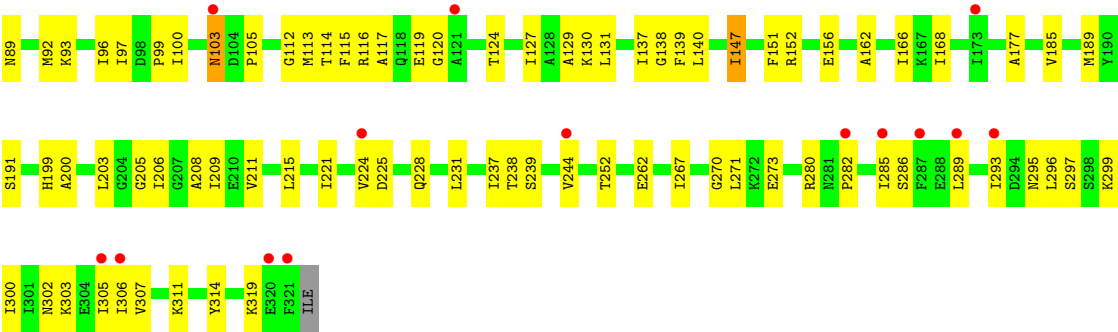


• Molecule 1: Basic membrane protein A



• Molecule 1: Basic membrane protein A





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.27Å 133.17Å 191.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.60 – 2.58 50.60 – 2.58	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.60-2.58) 93.7 (50.60-2.58)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.254 , 0.308 0.254 , 0.306	Depositor DCC
R_{free} test set	4093 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14665	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, THM, SO4, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.16	0/2457	0.34	0/3311
1	B	0.13	0/2457	0.31	0/3311
1	C	0.13	0/2457	0.31	0/3311
1	D	0.13	0/2457	0.33	0/3311
1	E	0.17	0/2457	0.37	0/3311
1	F	0.12	0/2457	0.31	0/3311
All	All	0.14	0/14742	0.33	0/19866

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2415	0	2418	70	0
1	B	2415	0	2418	62	0
1	C	2415	0	2418	56	0
1	D	2415	0	2418	75	0
1	E	2415	0	2418	63	0
1	F	2415	0	2418	74	0
2	A	17	0	14	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	17	0	14	0	0
2	C	17	0	14	0	0
2	D	17	0	14	0	0
2	E	17	0	14	0	0
2	F	17	0	14	0	0
3	A	5	0	0	1	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	F	4	0	3	0	0
6	A	19	0	0	0	0
6	B	13	0	0	1	0
6	C	5	0	0	0	0
6	D	8	0	0	0	0
6	E	3	0	0	0	0
6	F	14	0	0	0	0
All	All	14665	0	14595	384	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (384) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:TYR:HB3	1:E:275:VAL:HG21	1.59	0.85
1:A:39:LYS:HZ3	1:B:21:THR:HG23	1.49	0.77
1:F:300:ILE:HG22	1:F:305:ILE:HB	1.66	0.76
1:D:252:THR:HG23	1:D:253:SER:N	1.99	0.76
1:D:214:GLU:N	1:D:214:GLU:OE1	2.19	0.75
1:A:21:THR:HG22	1:A:23:ASP:H	1.53	0.73
1:D:281:ASN:HB3	1:D:285:ILE:HD13	1.69	0.73
1:D:73:LEU:HB2	1:D:96:ILE:HD12	1.71	0.72
1:B:60:LEU:HD21	1:B:73:LEU:HD21	1.69	0.72
1:F:74:ILE:HA	1:F:97:ILE:HB	1.71	0.72
1:D:13:LYS:HG2	1:D:45:GLU:HB2	1.70	0.72
1:B:153:TYR:HD1	1:B:314:TYR:HD2	1.37	0.71
1:D:295:ASN:O	1:D:299:LYS:N	2.24	0.71
1:B:73:LEU:HB2	1:B:96:ILE:HD12	1.73	0.70
1:F:56:TYR:HB3	1:F:81:VAL:HG11	1.72	0.70
1:E:246:ARG:O	1:E:250:ILE:HG13	1.91	0.70
1:C:56:TYR:HB3	1:C:81:VAL:HG11	1.74	0.69
1:D:252:THR:HG23	1:D:253:SER:H	1.57	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:HIS:ND1	1:A:260:THR:O	2.28	0.67
1:D:39:LYS:HG2	1:D:44:ILE:HD11	1.77	0.67
1:F:127:ILE:HD11	1:F:293:ILE:HG13	1.77	0.66
1:A:48:LEU:HB3	1:B:48:LEU:HB3	1.77	0.66
1:C:131:LEU:HD23	1:C:237:ILE:HD13	1.77	0.65
1:F:289:LEU:O	1:F:293:ILE:HG12	1.97	0.65
1:A:83:LYS:NZ	1:A:104:ASP:OD2	2.29	0.65
1:F:224:VAL:H	1:F:228:GLN:HE21	1.43	0.64
1:D:96:ILE:HG23	1:D:99:PRO:HG3	1.80	0.64
1:E:74:ILE:HA	1:E:97:ILE:HB	1.80	0.64
1:B:153:TYR:CD1	1:B:314:TYR:HD2	2.17	0.63
1:D:299:LYS:HB3	1:D:305:ILE:HD12	1.81	0.63
1:E:41:GLU:OE1	1:E:42:PHE:HD2	1.79	0.63
1:C:173:ILE:HD11	1:C:201:ALA:HB1	1.81	0.63
1:F:26:SER:HB2	1:F:225:ASP:HB2	1.79	0.63
1:F:99:PRO:HD2	1:F:114:THR:HG22	1.81	0.63
1:B:35:VAL:HG11	1:B:46:LEU:HD13	1.80	0.63
1:A:76:TYR:HB2	1:A:100:ILE:HG12	1.81	0.62
1:C:289:LEU:O	1:C:293:ILE:HG12	1.99	0.62
1:D:127:ILE:HD11	1:D:293:ILE:HG13	1.82	0.62
1:D:252:THR:CG2	1:D:253:SER:H	2.12	0.62
1:F:49:LYS:NZ	1:F:50:GLU:O	2.31	0.62
1:A:273:GLU:OE1	1:A:273:GLU:N	2.33	0.62
1:B:285:ILE:HG23	1:B:289:LEU:HD23	1.81	0.62
1:D:252:THR:CG2	1:D:253:SER:N	2.63	0.61
1:A:77:ARG:NH2	3:A:402:SO4:O4	2.32	0.61
1:D:74:ILE:HA	1:D:97:ILE:HB	1.81	0.61
1:D:249:ASN:O	1:D:252:THR:HG22	2.00	0.61
1:A:295:ASN:O	1:A:299:LYS:N	2.31	0.61
1:E:48:LEU:HB3	1:F:48:LEU:HB3	1.83	0.61
1:B:21:THR:HG22	1:B:23:ASP:H	1.66	0.60
1:E:42:PHE:CE1	1:E:256:LEU:HB3	2.36	0.60
1:B:300:ILE:HG22	1:B:305:ILE:HB	1.84	0.60
1:A:21:THR:HG23	1:B:39:LYS:HE3	1.83	0.59
1:D:116:ARG:HE	1:D:270:GLY:HA3	1.66	0.59
1:F:293:ILE:HA	1:F:296:LEU:HB2	1.84	0.59
1:E:33:ASN:HA	1:E:36:LYS:HG2	1.85	0.59
1:B:56:TYR:HD2	1:B:81:VAL:HG21	1.67	0.59
1:D:32:LEU:O	1:D:36:LYS:HG2	2.03	0.59
1:D:295:ASN:HA	1:D:298:SER:HB3	1.85	0.59
1:C:71:ILE:HB	1:C:94:TYR:HD1	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:LEU:HD23	1:F:237:ILE:HD13	1.85	0.58
1:D:13:LYS:HB2	1:D:68:SER:HA	1.85	0.58
1:F:33:ASN:HA	1:F:36:LYS:HG2	1.85	0.58
1:F:156:GLU:HG2	1:F:168:ILE:HG21	1.86	0.58
1:D:17:ILE:HD11	1:D:51:SER:HB3	1.86	0.58
1:A:74:ILE:HA	1:A:97:ILE:HB	1.86	0.58
1:B:18:ILE:HG22	1:B:74:ILE:HD11	1.84	0.58
1:B:153:TYR:HD1	1:B:314:TYR:CD2	2.20	0.57
1:C:152:ARG:HD2	1:C:170:THR:HG21	1.86	0.57
1:F:199:HIS:ND1	1:F:205:GLY:HA3	2.19	0.57
1:E:41:GLU:OE1	1:E:42:PHE:CD2	2.58	0.57
1:F:51:SER:OG	1:F:59:ASP:OD2	2.21	0.57
1:A:280:ARG:HH22	1:F:282:PRO:HA	1.69	0.57
1:F:73:LEU:HB2	1:F:96:ILE:HD12	1.86	0.57
1:A:128:ALA:HB2	1:A:222:ILE:HD11	1.86	0.57
1:D:38:VAL:HG21	1:D:252:THR:CG2	2.35	0.57
1:F:25:LYS:HG3	1:F:206:ILE:HD11	1.86	0.57
1:C:311:LYS:O	1:C:315:GLU:HG2	2.05	0.57
1:C:300:ILE:HG22	1:C:305:ILE:HG13	1.86	0.56
1:F:200:ALA:HA	1:F:224:VAL:HG21	1.86	0.56
1:B:18:ILE:HA	1:B:74:ILE:HD11	1.87	0.56
1:D:117:ALA:HB1	1:D:151:PHE:CE1	2.40	0.56
1:F:271:LEU:HD22	1:F:300:ILE:HD11	1.88	0.56
1:B:74:ILE:HA	1:B:97:ILE:HB	1.86	0.56
1:C:122:PHE:HE1	1:C:296:LEU:HD13	1.71	0.56
1:E:273:GLU:N	1:E:273:GLU:OE1	2.39	0.56
1:C:183:ARG:NH2	1:C:214:GLU:OE2	2.39	0.56
1:D:152:ARG:HH11	1:D:170:THR:HG21	1.71	0.56
1:D:84:VAL:HA	1:D:87:LEU:HG	1.88	0.56
1:D:15:SER:HB3	1:D:63:LEU:HD13	1.87	0.55
1:D:140:LEU:HD13	1:D:185:VAL:HG11	1.89	0.55
1:E:21:THR:O	1:E:28:ASN:ND2	2.39	0.55
1:B:69:ASP:OD1	1:B:255:HIS:NE2	2.40	0.55
1:A:123:LEU:HD21	1:A:297:SER:HB3	1.89	0.55
1:F:96:ILE:HG22	1:F:112:GLY:HA2	1.88	0.55
1:F:18:ILE:HD11	1:F:50:GLU:HG2	1.87	0.54
1:F:38:VAL:HG21	1:F:252:THR:HB	1.88	0.54
1:A:289:LEU:O	1:A:293:ILE:HG12	2.06	0.54
1:C:220:TYR:HB3	1:C:237:ILE:HG13	1.88	0.54
1:C:296:LEU:O	1:C:300:ILE:HG23	2.07	0.54
1:B:212:ALA:O	1:B:235:ASN:ND2	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:VAL:HG11	1:E:46:LEU:HD13	1.88	0.54
1:F:237:ILE:HG22	1:F:238:THR:HG22	1.89	0.54
1:F:209:ILE:HD13	1:F:221:ILE:HD12	1.90	0.54
1:B:147:ILE:HD12	1:B:148:VAL:N	2.22	0.54
1:A:116:ARG:HH21	1:A:270:GLY:HA3	1.73	0.54
1:E:101:TYR:HB3	1:E:106:ILE:HD11	1.89	0.53
1:A:60:LEU:HD11	1:A:73:LEU:HD21	1.89	0.53
1:B:273:GLU:N	1:B:273:GLU:OE1	2.40	0.53
1:E:26:SER:O	1:E:28:ASN:N	2.42	0.53
1:B:258:THR:HG22	1:C:144:GLU:HB3	1.91	0.53
1:A:289:LEU:O	1:A:293:ILE:N	2.37	0.53
1:F:92:MET:HE3	1:F:93:LYS:H	1.73	0.53
1:A:280:ARG:HH12	1:F:282:PRO:HA	1.72	0.53
1:E:83:LYS:NZ	1:E:104:ASP:OD2	2.34	0.53
1:E:209:ILE:HG13	1:E:221:ILE:HG21	1.90	0.53
1:E:50:GLU:OE1	1:F:39:LYS:NZ	2.42	0.53
1:A:83:LYS:O	1:A:87:LEU:HD22	2.09	0.52
1:F:238:THR:OG1	1:F:239:SER:N	2.42	0.52
1:A:50:GLU:OE1	1:B:46:LEU:N	2.29	0.52
1:E:123:LEU:HG	1:E:293:ILE:HG23	1.92	0.52
1:B:163:ASN:HB3	1:B:166:ILE:HB	1.91	0.52
1:D:238:THR:OG1	1:D:239:SER:N	2.43	0.52
1:F:35:VAL:HG11	1:F:46:LEU:HD13	1.92	0.52
1:E:151:PHE:HE1	1:E:224:VAL:CG2	2.22	0.52
1:F:73:LEU:HB2	1:F:96:ILE:CD1	2.39	0.52
1:A:281:ASN:ND2	1:A:283:LYS:HD2	2.24	0.52
1:B:93:LYS:HB3	1:B:261:PHE:CE2	2.44	0.52
1:B:177:ALA:HA	1:B:203:LEU:HB2	1.91	0.52
1:C:71:ILE:HB	1:C:94:TYR:CD1	2.45	0.51
1:B:314:TYR:HE1	1:B:318:LEU:HD11	1.76	0.51
1:D:152:ARG:NE	1:D:172:TYR:OH	2.42	0.51
1:E:289:LEU:HA	1:E:292:GLU:OE2	2.10	0.51
1:D:35:VAL:HG13	1:D:46:LEU:HD21	1.92	0.51
1:B:137:ILE:HG22	1:B:196:ILE:HB	1.93	0.51
1:F:140:LEU:HD23	1:F:185:VAL:HG11	1.92	0.51
1:B:99:PRO:HD2	1:B:114:THR:HG22	1.93	0.51
1:C:271:LEU:HD12	1:C:300:ILE:HD11	1.91	0.51
1:D:249:ASN:HA	1:D:252:THR:HG22	1.93	0.51
1:C:42:PHE:CD2	1:C:256:LEU:HD23	2.46	0.51
1:B:116:ARG:HB3	1:B:119:GLU:HG3	1.93	0.51
1:A:163:ASN:HB3	1:A:166:ILE:HB	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:TRP:CZ3	1:C:113:MET:HE1	2.46	0.50
1:D:104:ASP:OD1	1:D:104:ASP:N	2.39	0.50
1:D:289:LEU:O	1:D:293:ILE:HG12	2.10	0.50
1:E:98:ASP:OD2	1:E:242:LYS:NZ	2.44	0.50
1:A:129:ALA:HB3	1:A:162:ALA:HB3	1.93	0.50
1:B:18:ILE:HD11	1:B:50:GLU:HG2	1.93	0.50
1:E:282:PRO:C	1:E:284:MET:H	2.20	0.50
1:C:9:SER:C	1:C:11:ILE:H	2.20	0.50
1:C:128:ALA:HB2	1:C:222:ILE:HD11	1.94	0.50
1:E:248:LEU:O	1:E:252:THR:HG22	2.12	0.50
1:B:128:ALA:HB2	1:B:222:ILE:HD11	1.94	0.49
1:D:249:ASN:C	1:D:252:THR:HG22	2.37	0.49
1:A:294:ASP:O	1:A:296:LEU:N	2.42	0.49
1:C:119:GLU:HB3	1:C:271:LEU:HG	1.93	0.49
1:E:38:VAL:HG11	1:E:252:THR:HG23	1.94	0.49
1:C:199:HIS:CE1	1:C:205:GLY:HA3	2.47	0.49
1:A:38:VAL:HG21	1:A:252:THR:HG23	1.94	0.49
1:A:292:GLU:O	1:A:296:LEU:HB2	2.13	0.49
1:C:160:LYS:HG2	1:C:318:LEU:HD21	1.94	0.49
1:F:302:ASN:O	1:F:303:LYS:HG3	2.13	0.49
1:A:199:HIS:HD2	1:A:201:ALA:H	1.60	0.49
1:A:288:GLU:O	1:A:289:LEU:HB3	2.13	0.48
1:D:80:ASP:O	1:D:84:VAL:HG13	2.13	0.48
1:B:173:ILE:HD11	1:B:201:ALA:HB1	1.94	0.48
1:D:198:HIS:NE2	1:D:240:THR:OG1	2.45	0.48
1:E:38:VAL:HG11	1:E:252:THR:CG2	2.43	0.48
1:F:35:VAL:O	1:F:38:VAL:HG12	2.13	0.48
1:C:32:LEU:O	1:C:36:LYS:HG2	2.14	0.48
1:C:136:LYS:HB3	1:C:194:ILE:HD13	1.95	0.48
1:E:295:ASN:C	1:E:295:ASN:HD22	2.21	0.48
1:A:224:VAL:N	1:A:228:GLN:OE1	2.29	0.48
1:D:237:ILE:HG22	1:D:238:THR:HG22	1.94	0.48
1:B:32:LEU:O	1:B:36:LYS:HG2	2.12	0.48
1:F:18:ILE:HG22	1:F:74:ILE:HD11	1.95	0.48
1:D:129:ALA:HB3	1:D:162:ALA:HB3	1.96	0.48
1:A:237:ILE:HG22	1:A:238:THR:HG22	1.95	0.48
1:A:248:LEU:O	1:A:252:THR:HG22	2.14	0.48
1:B:35:VAL:O	1:B:38:VAL:HG12	2.13	0.48
1:D:38:VAL:HG21	1:D:252:THR:HG21	1.95	0.48
1:D:76:TYR:O	1:D:79:SER:OG	2.30	0.48
1:A:39:LYS:NZ	1:B:50:GLU:OE2	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:HG3	1:A:250:ILE:HD12	1.96	0.47
1:F:116:ARG:NH2	1:F:119:GLU:OE1	2.47	0.47
1:A:290:GLU:HG3	1:F:280:ARG:HH21	1.79	0.47
1:D:271:LEU:HD22	1:D:300:ILE:HD11	1.95	0.47
1:E:121:ALA:HA	1:E:124:THR:HG22	1.97	0.47
1:F:24:ASP:OD1	1:F:24:ASP:N	2.44	0.47
1:F:177:ALA:HA	1:F:203:LEU:HB2	1.97	0.47
1:A:104:ASP:OD1	1:A:104:ASP:N	2.46	0.47
1:C:74:ILE:HA	1:C:97:ILE:HG12	1.96	0.47
1:E:232:ALA:O	1:E:236:VAL:HG23	2.14	0.47
1:B:129:ALA:HB3	1:B:162:ALA:HB3	1.95	0.47
1:A:269:TYR:CD2	1:A:275:VAL:HG21	2.49	0.47
1:E:72:TRP:HH2	1:E:113:MET:HE3	1.80	0.47
1:B:147:ILE:HD12	1:B:148:VAL:H	1.79	0.47
1:B:152:ARG:O	1:B:156:GLU:HG3	2.15	0.47
1:D:177:ALA:HA	1:D:203:LEU:HD12	1.97	0.47
1:B:310:ASN:HD21	1:B:312:GLU:HB2	1.79	0.47
1:C:269:TYR:CD1	1:C:275:VAL:HG21	2.50	0.47
1:D:35:VAL:CG1	1:D:46:LEU:HD21	2.44	0.47
1:D:213:LYS:HE2	1:D:213:LYS:HB3	1.80	0.47
1:F:18:ILE:HA	1:F:74:ILE:HD11	1.96	0.47
1:E:288:GLU:OE2	1:E:288:GLU:N	2.19	0.47
1:F:139:PHE:CE1	1:F:152:ARG:HA	2.50	0.47
1:B:271:LEU:HD22	1:B:300:ILE:HD11	1.96	0.47
1:C:185:VAL:O	1:C:189:MET:HG3	2.15	0.47
1:F:224:VAL:HG12	1:F:228:GLN:HE22	1.79	0.47
1:F:129:ALA:HB3	1:F:162:ALA:HB3	1.96	0.46
1:E:111:VAL:HG11	1:E:251:PHE:CZ	2.51	0.46
1:A:103:ASN:OD1	1:A:103:ASN:N	2.49	0.46
1:A:152:ARG:HD3	1:A:170:THR:HG21	1.97	0.46
1:B:141:GLY:O	1:B:173:ILE:HG12	2.16	0.46
1:C:224:VAL:O	1:C:226:GLU:N	2.43	0.46
1:E:234:ASP:OD1	1:E:234:ASP:N	2.49	0.46
1:F:208:ALA:O	1:F:211:VAL:HG12	2.16	0.46
1:C:74:ILE:HG22	1:C:97:ILE:HD11	1.97	0.46
1:D:137:ILE:HG22	1:D:196:ILE:HB	1.98	0.46
1:A:139:PHE:CD1	1:A:152:ARG:HG2	2.51	0.46
1:B:42:PHE:HZ	1:B:257:LYS:HG3	1.81	0.46
1:D:224:VAL:O	1:D:226:GLU:N	2.47	0.46
1:C:305:ILE:O	1:C:306:ILE:HD12	2.16	0.46
1:C:17:ILE:HD12	1:C:17:ILE:HA	1.83	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:LEU:HD11	1:D:271:LEU:HD21	1.97	0.46
1:E:93:LYS:HB3	1:E:261:PHE:CE1	2.51	0.46
1:A:36:LYS:HB3	1:B:22:PHE:CZ	2.51	0.46
1:E:23:ASP:CG	1:F:36:LYS:HD3	2.41	0.46
1:A:173:ILE:HG13	1:A:175:SER:H	1.81	0.45
1:A:281:ASN:OD1	1:A:284:MET:HG3	2.15	0.45
1:B:56:TYR:HB3	1:B:81:VAL:HG11	1.98	0.45
1:B:271:LEU:HD23	1:B:301:ILE:HG13	1.97	0.45
1:C:19:ASP:OD2	1:C:56:TYR:OH	2.22	0.45
1:E:43:LYS:HB2	1:E:43:LYS:HE2	1.62	0.45
1:F:137:ILE:HG12	1:F:166:ILE:HD11	1.98	0.45
1:F:285:ILE:HG23	1:F:289:LEU:HD23	1.98	0.45
1:B:228:GLN:NE2	6:B:501:HOH:O	2.48	0.45
1:F:147:ILE:H	1:F:147:ILE:HG13	1.54	0.45
1:D:136:LYS:NZ	1:D:193:GLU:HB2	2.31	0.45
1:F:26:SER:O	1:F:28:ASN:N	2.50	0.45
1:A:26:SER:HB2	1:A:225:ASP:HB2	1.99	0.45
1:B:294:ASP:HB3	1:E:291:LYS:NZ	2.32	0.45
1:D:299:LYS:HD3	1:D:305:ILE:HD11	1.97	0.45
1:D:314:TYR:CZ	1:D:318:LEU:HD11	2.51	0.45
1:E:24:ASP:OD1	1:E:24:ASP:N	2.50	0.45
1:E:116:ARG:CZ	1:E:270:GLY:HA3	2.46	0.45
1:D:136:LYS:HB2	1:D:136:LYS:HE3	1.71	0.45
1:F:117:ALA:HB1	1:F:151:PHE:CE1	2.52	0.45
1:F:127:ILE:CD1	1:F:293:ILE:HG13	2.43	0.45
1:A:26:SER:O	1:A:28:ASN:N	2.50	0.45
1:F:295:ASN:O	1:F:299:LYS:HB2	2.16	0.45
1:D:311:LYS:HG2	1:D:312:GLU:N	2.30	0.45
1:E:28:ASN:OD1	1:E:74:ILE:HD11	2.17	0.45
1:A:190:TYR:HD1	1:A:215:LEU:HD12	1.81	0.45
1:D:249:ASN:HA	1:D:252:THR:CG2	2.47	0.45
1:D:292:GLU:O	1:D:296:LEU:HB2	2.17	0.45
1:F:16:LEU:HD12	1:F:72:TRP:HB2	1.99	0.44
1:A:238:THR:OG1	1:A:239:SER:N	2.50	0.44
1:D:195:ASP:N	1:D:195:ASP:OD2	2.49	0.44
1:D:220:TYR:C	1:D:221:ILE:HD12	2.42	0.44
1:E:73:LEU:O	1:E:96:ILE:HD12	2.18	0.44
1:F:270:GLY:N	1:F:273:GLU:OE2	2.49	0.44
1:B:117:ALA:HB1	1:B:151:PHE:CE1	2.52	0.44
1:F:224:VAL:N	1:F:228:GLN:HE21	2.13	0.44
1:A:258:THR:OG1	1:A:260:THR:OG1	2.26	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:GLY:HA3	1:F:189:MET:HE2	1.99	0.44
1:C:152:ARG:HH11	1:C:170:THR:HG21	1.83	0.44
1:C:129:ALA:HB3	1:C:162:ALA:HB3	2.00	0.44
1:D:288:GLU:HA	1:D:291:LYS:HB3	1.98	0.44
1:A:35:VAL:O	1:A:38:VAL:HG12	2.18	0.44
1:A:56:TYR:HB3	1:A:81:VAL:HG21	2.00	0.44
1:C:32:LEU:HD13	1:C:48:LEU:HD21	2.00	0.44
1:D:199:HIS:CE1	1:D:205:GLY:HA3	2.53	0.43
1:D:207:GLY:O	1:D:210:GLU:HB2	2.18	0.43
1:F:311:LYS:O	1:F:314:TYR:HB3	2.18	0.43
1:B:156:GLU:HG2	1:B:168:ILE:HG21	2.01	0.43
1:C:76:TYR:HD1	1:C:76:TYR:H	1.64	0.43
1:C:144:GLU:HG3	1:C:172:TYR:CZ	2.53	0.43
1:A:123:LEU:HG	1:A:293:ILE:HG23	1.99	0.43
1:A:281:ASN:HD21	1:A:283:LYS:HD2	1.83	0.43
1:D:210:GLU:O	1:D:214:GLU:OE1	2.37	0.43
1:A:183:ARG:NH2	1:A:214:GLU:OE2	2.52	0.43
1:A:289:LEU:HA	1:A:292:GLU:HB2	1.99	0.43
1:E:72:TRP:CH2	1:E:248:LEU:HA	2.53	0.43
1:F:130:LYS:HG2	1:F:162:ALA:HB1	2.00	0.43
1:A:283:LYS:HD2	1:A:283:LYS:H	1.82	0.43
1:E:106:ILE:HG22	1:E:264:GLY:HA2	2.01	0.43
1:C:73:LEU:HB2	1:C:96:ILE:HG13	1.99	0.43
1:D:19:ASP:OD2	1:D:56:TYR:OH	2.35	0.43
1:D:269:TYR:CD1	1:D:275:VAL:HG21	2.54	0.43
1:A:16:LEU:HD12	1:A:72:TRP:HB2	2.01	0.43
1:A:115:PHE:CZ	1:A:244:VAL:HG12	2.54	0.43
1:C:73:LEU:HD22	1:C:82:ALA:HB2	2.01	0.43
1:E:129:ALA:HB3	1:E:162:ALA:HB3	2.01	0.43
1:A:19:ASP:OD1	1:A:19:ASP:N	2.52	0.43
1:D:38:VAL:HG21	1:D:252:THR:HG23	2.01	0.43
1:D:164:LYS:HD2	1:D:321:PHE:HE2	1.84	0.43
1:E:36:LYS:HD3	1:F:23:ASP:CG	2.44	0.43
1:E:151:PHE:HE1	1:E:224:VAL:HG23	1.83	0.43
1:E:159:ALA:HB1	1:E:166:ILE:HG21	1.99	0.43
1:A:106:ILE:HG23	1:A:110:LEU:HD23	2.01	0.42
1:C:14:VAL:O	1:C:46:LEU:HA	2.18	0.42
1:C:73:LEU:O	1:C:96:ILE:HA	2.19	0.42
1:C:177:ALA:HA	1:C:203:LEU:HB2	2.01	0.42
1:D:49:LYS:HA	1:D:49:LYS:HD2	1.87	0.42
1:D:76:TYR:H	1:D:76:TYR:HD1	1.65	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:THR:O	1:E:276:VAL:HA	2.18	0.42
1:A:130:LYS:HG2	1:A:162:ALA:HB1	2.01	0.42
1:B:16:LEU:O	1:B:48:LEU:HA	2.18	0.42
1:C:60:LEU:HD23	1:C:60:LEU:HA	1.84	0.42
1:C:207:GLY:HA2	1:C:210:GLU:OE2	2.18	0.42
1:D:57:LEU:HD12	1:D:57:LEU:H	1.84	0.42
1:E:282:PRO:C	1:E:284:MET:N	2.76	0.42
1:B:139:PHE:C	1:B:139:PHE:CD2	2.97	0.42
1:D:199:HIS:ND1	1:D:205:GLY:HA3	2.34	0.42
1:F:37:LYS:HE3	1:F:37:LYS:HB2	1.77	0.42
1:F:103:ASN:HB2	1:F:105:PRO:HD2	2.01	0.42
1:A:9:SER:O	1:A:10:GLU:HG2	2.18	0.42
1:A:42:PHE:HB3	1:A:44:ILE:HG23	2.01	0.42
1:B:139:PHE:HE2	1:B:141:GLY:HA3	1.84	0.42
1:B:242:LYS:HG3	1:B:276:VAL:HG12	2.02	0.42
1:B:294:ASP:OD1	1:E:287:PHE:CE1	2.73	0.42
1:B:198:HIS:NE2	1:B:240:THR:OG1	2.48	0.42
1:C:271:LEU:HD23	1:C:271:LEU:HA	1.89	0.42
1:D:35:VAL:O	1:D:38:VAL:HG12	2.20	0.42
1:E:34:GLY:O	1:E:38:VAL:HG22	2.19	0.42
1:E:107:PRO:HG2	1:E:110:LEU:HB3	2.01	0.42
1:B:164:LYS:HD3	1:B:164:LYS:N	2.35	0.42
1:C:215:LEU:HB3	1:C:219:HIS:CE1	2.55	0.42
1:D:18:ILE:HD11	1:D:50:GLU:HG2	2.01	0.42
1:E:104:ASP:OD1	1:E:104:ASP:N	2.51	0.42
1:F:96:ILE:HG21	1:F:99:PRO:HB3	2.02	0.42
1:E:197:ILE:HB	1:E:221:ILE:HD13	2.02	0.42
1:B:136:LYS:HB2	1:B:136:LYS:HE2	1.75	0.42
1:C:32:LEU:HG	1:C:36:LYS:HE3	2.02	0.42
1:E:122:PHE:CD1	1:E:158:GLY:HA2	2.54	0.42
1:F:209:ILE:HA	1:F:221:ILE:HD12	2.00	0.42
1:F:319:LYS:HA	1:F:319:LYS:HD2	1.91	0.42
1:A:215:LEU:HB3	1:A:219:HIS:CE1	2.54	0.41
1:B:178:ASP:O	1:B:180:GLU:N	2.50	0.41
1:C:72:TRP:HZ3	1:C:113:MET:HE1	1.85	0.41
1:E:143:ILE:H	1:E:143:ILE:HG13	1.64	0.41
1:C:74:ILE:HD12	1:C:74:ILE:O	2.20	0.41
1:A:209:ILE:HG13	1:A:221:ILE:HD13	2.02	0.41
1:D:127:ILE:HG23	1:D:131:LEU:HD22	2.02	0.41
1:C:23:ASP:N	1:C:23:ASP:OD1	2.53	0.41
1:F:199:HIS:HD1	1:F:205:GLY:HA3	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:VAL:O	1:F:215:LEU:HG	2.20	0.41
1:D:138:GLY:HA3	1:D:189:MET:HE2	2.02	0.41
1:E:104:ASP:HA	1:E:105:PRO:HD2	1.89	0.41
1:C:152:ARG:HH21	1:C:153:TYR:HE1	1.69	0.41
1:E:72:TRP:CH2	1:E:113:MET:HE3	2.55	0.41
1:E:115:PHE:HB2	1:E:242:LYS:HE2	2.02	0.41
1:F:113:MET:SD	1:F:267:ILE:HD12	2.61	0.41
1:C:212:ALA:O	1:C:235:ASN:ND2	2.53	0.41
1:C:315:GLU:HG2	1:C:315:GLU:H	1.72	0.41
1:E:126:TYR:CZ	1:E:130:LYS:HE3	2.56	0.41
1:E:168:ILE:HD12	1:E:168:ILE:O	2.20	0.41
1:A:60:LEU:HD23	1:A:60:LEU:HA	1.88	0.41
1:A:190:TYR:CD1	1:A:215:LEU:HD12	2.55	0.41
1:A:286:SER:OG	1:A:288:GLU:O	2.36	0.41
1:B:199:HIS:ND1	1:B:205:GLY:HA3	2.36	0.41
1:B:299:LYS:HA	1:B:299:LYS:HD3	1.87	0.41
1:C:35:VAL:O	1:C:38:VAL:HG12	2.20	0.41
1:D:97:ILE:HD13	1:D:113:MET:HB2	2.03	0.41
1:D:103:ASN:OD1	1:D:103:ASN:N	2.43	0.41
1:E:21:THR:HG22	1:E:23:ASP:H	1.84	0.41
1:A:72:TRP:CH2	1:A:248:LEU:HA	2.56	0.41
1:B:199:HIS:NE2	1:B:228:GLN:OE1	2.34	0.40
1:C:26:SER:HB2	1:C:225:ASP:HB2	2.02	0.40
1:D:56:TYR:HB3	1:D:81:VAL:HG11	2.01	0.40
1:C:63:LEU:HB3	1:C:71:ILE:HD12	2.03	0.40
1:F:64:LYS:NZ	1:F:89:ASN:OD1	2.54	0.40
1:F:115:PHE:CE2	1:F:244:VAL:HG12	2.57	0.40
1:D:285:ILE:HG21	1:D:290:GLU:HG2	2.02	0.40
1:E:122:PHE:HD2	1:E:307:VAL:HG22	1.86	0.40
1:A:118:GLN:O	1:A:307:VAL:HG11	2.21	0.40
1:B:152:ARG:NE	1:B:156:GLU:OE2	2.43	0.40
1:E:15:SER:HB2	1:E:71:ILE:HG12	2.03	0.40
1:F:96:ILE:HD12	1:F:96:ILE:HA	1.86	0.40
1:F:113:MET:HE2	1:F:113:MET:HB2	1.90	0.40
1:F:228:GLN:HB3	1:F:231:LEU:HD12	2.03	0.40
1:A:32:LEU:O	1:A:36:LYS:HG2	2.22	0.40
1:E:237:ILE:HA	1:E:284:MET:HG2	2.03	0.40
1:F:120:GLY:O	1:F:124:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	311/328 (95%)	291 (94%)	18 (6%)	2 (1%)	21	39
1	B	311/328 (95%)	291 (94%)	18 (6%)	2 (1%)	21	39
1	C	311/328 (95%)	292 (94%)	15 (5%)	4 (1%)	9	19
1	D	311/328 (95%)	289 (93%)	21 (7%)	1 (0%)	36	56
1	E	311/328 (95%)	289 (93%)	18 (6%)	4 (1%)	9	19
1	F	311/328 (95%)	294 (94%)	14 (4%)	3 (1%)	12	26
All	All	1866/1968 (95%)	1746 (94%)	104 (6%)	16 (1%)	14	29

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	283	LYS
1	C	289	LEU
1	E	27	PHE
1	F	307	VAL
1	A	27	PHE
1	B	101	TYR
1	C	227	ASP
1	F	27	PHE
1	C	143	ILE
1	D	306	ILE
1	E	103	ASN
1	F	262	GLU
1	B	284	MET
1	A	262	GLU
1	E	306	ILE
1	C	105	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/270 (96%)	251 (97%)	7 (3%)	39	65
1	B	258/270 (96%)	251 (97%)	7 (3%)	39	65
1	C	258/270 (96%)	247 (96%)	11 (4%)	26	49
1	D	258/270 (96%)	251 (97%)	7 (3%)	39	65
1	E	258/270 (96%)	247 (96%)	11 (4%)	26	49
1	F	258/270 (96%)	247 (96%)	11 (4%)	26	49
All	All	1548/1620 (96%)	1494 (96%)	54 (4%)	32	57

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	81	VAL
1	A	119	GLU
1	A	170	THR
1	A	191	SER
1	A	276	VAL
1	A	298	SER
1	B	17	ILE
1	B	32	LEU
1	B	46	LEU
1	B	147	ILE
1	B	199	HIS
1	B	253	SER
1	B	321	PHE
1	C	35	VAL
1	C	38	VAL
1	C	48	LEU
1	C	217	SER
1	C	221	ILE
1	C	271	LEU
1	C	289	LEU
1	C	298	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	300	ILE
1	C	305	ILE
1	C	309	SER
1	D	35	VAL
1	D	131	LEU
1	D	133	LYS
1	D	179	LEU
1	D	199	HIS
1	D	238	THR
1	D	295	ASN
1	E	50	GLU
1	E	73	LEU
1	E	74	ILE
1	E	147	ILE
1	E	168	ILE
1	E	170	THR
1	E	191	SER
1	E	217	SER
1	E	249	ASN
1	E	289	LEU
1	E	298	SER
1	F	51	SER
1	F	55	SER
1	F	68	SER
1	F	73	LEU
1	F	100	ILE
1	F	103	ASN
1	F	147	ILE
1	F	191	SER
1	F	286	SER
1	F	297	SER
1	F	306	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	89	ASN
1	A	199	HIS
1	A	281	ASN
1	B	88	GLN
1	B	89	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	254	ASN
1	B	302	ASN
1	C	89	ASN
1	C	219	HIS
1	C	259	ASN
1	D	171	GLN
1	D	235	ASN
1	D	302	ASN
1	E	254	ASN
1	E	295	ASN
1	F	228	GLN
1	F	249	ASN
1	F	281	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ACT	F	402	-	3,3,3	1.41	1 (33%)	3,3,3	1.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	THM	E	401	-	18,18,18	0.16	0	26,26,26	0.24	0
2	THM	D	401	-	18,18,18	0.11	0	26,26,26	0.18	0
2	THM	F	401	-	18,18,18	0.09	0	26,26,26	0.17	0
2	THM	A	401	-	18,18,18	0.15	0	26,26,26	0.24	0
3	SO4	A	402	-	4,4,4	0.25	0	6,6,6	0.07	0
2	THM	C	401	-	18,18,18	0.13	0	26,26,26	0.23	0
2	THM	B	401	-	18,18,18	0.12	0	26,26,26	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	THM	E	401	-	-	0/6/18/18	0/2/2/2
2	THM	D	401	-	-	0/6/18/18	0/2/2/2
2	THM	F	401	-	-	2/6/18/18	0/2/2/2
2	THM	A	401	-	-	0/6/18/18	0/2/2/2
2	THM	C	401	-	-	0/6/18/18	0/2/2/2
2	THM	B	401	-	-	0/6/18/18	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	402	ACT	CH3-C	2.05	1.57	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

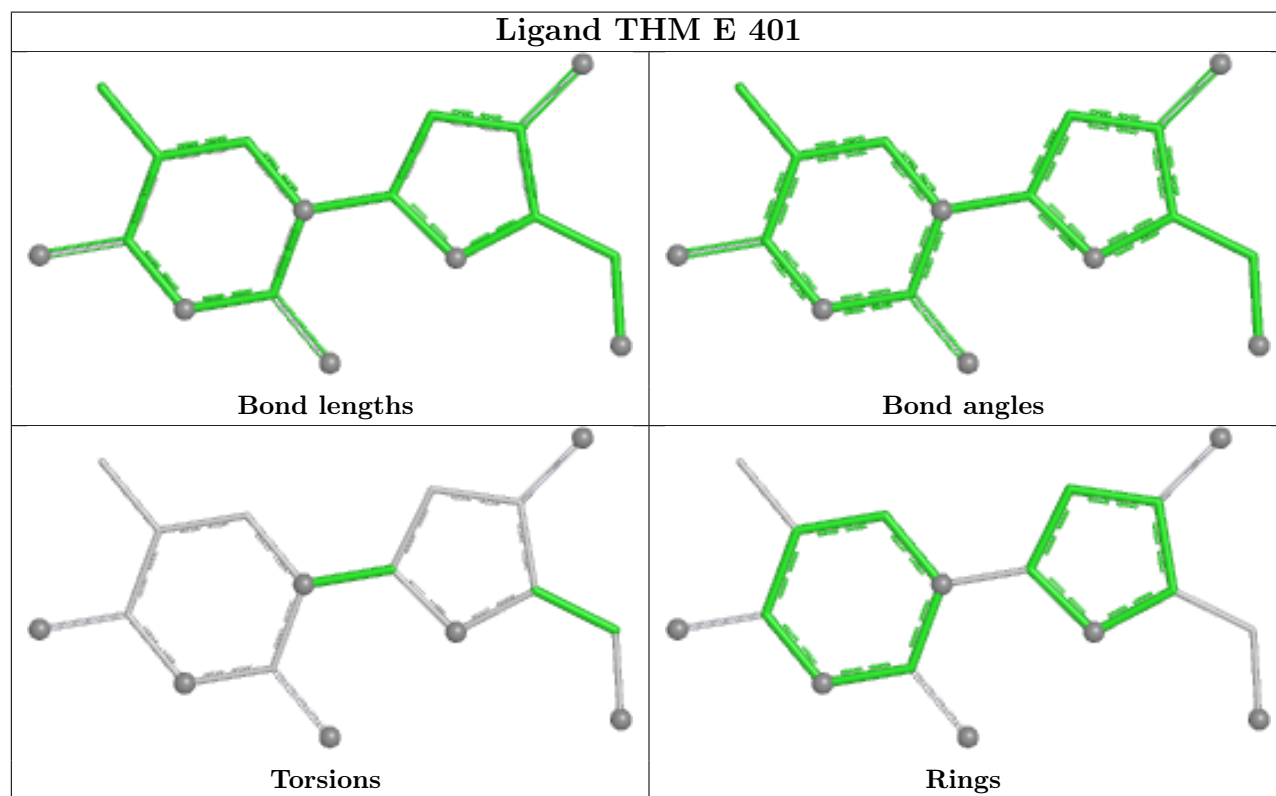
Mol	Chain	Res	Type	Atoms
2	F	401	THM	C3'-C4'-C5'-O5'
2	F	401	THM	O4'-C4'-C5'-O5'

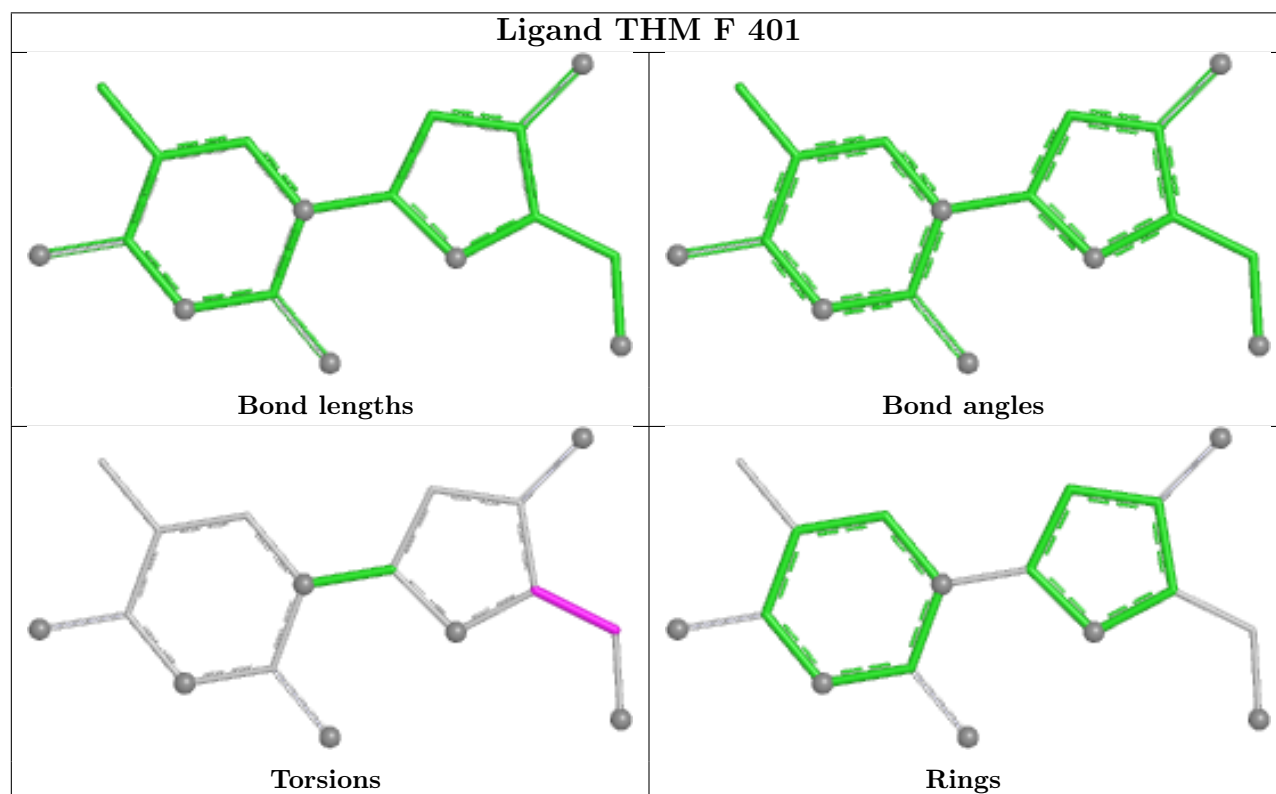
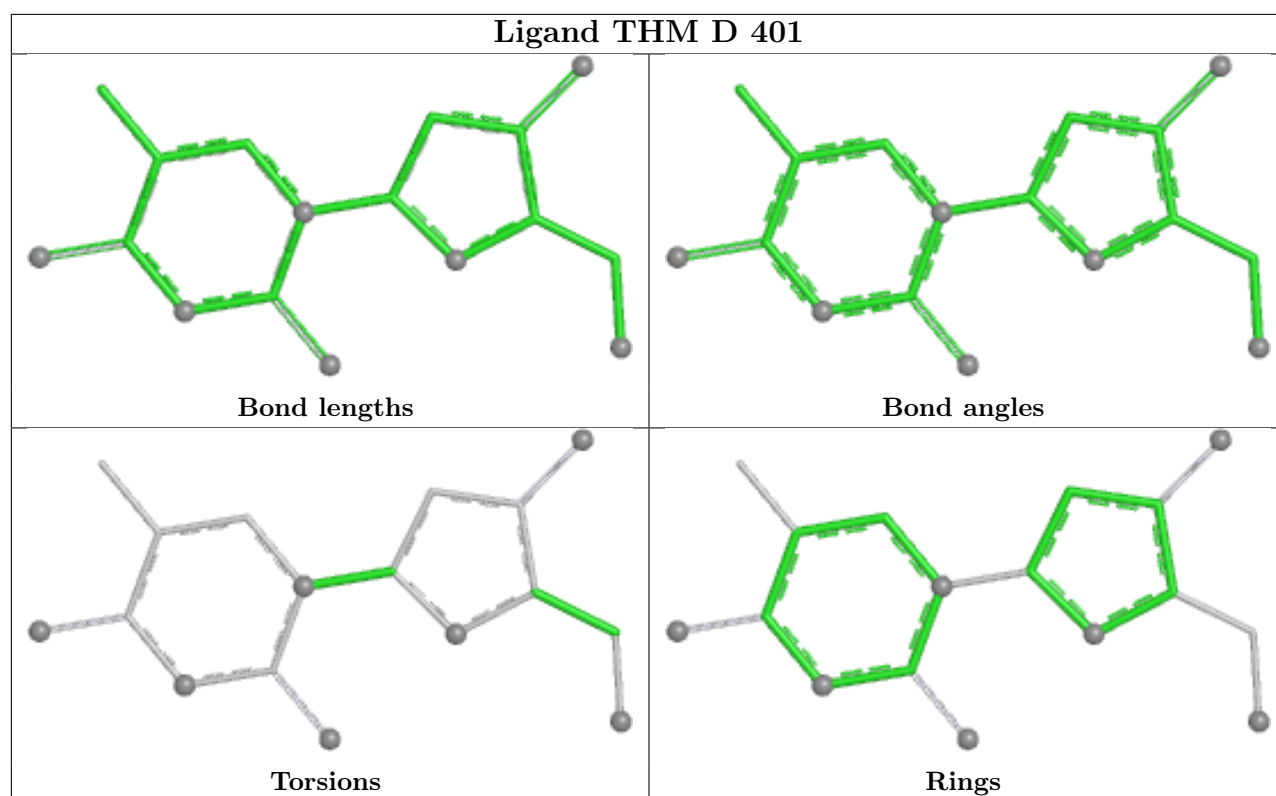
There are no ring outliers.

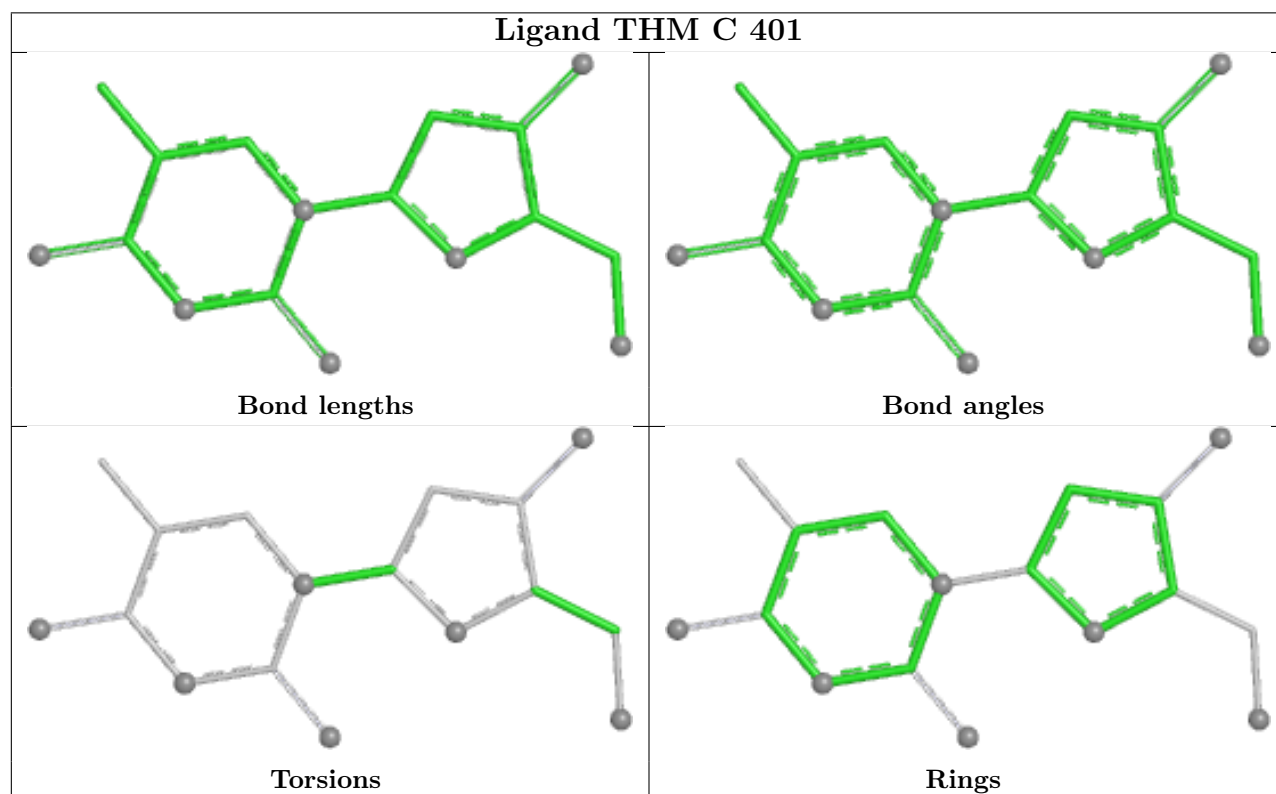
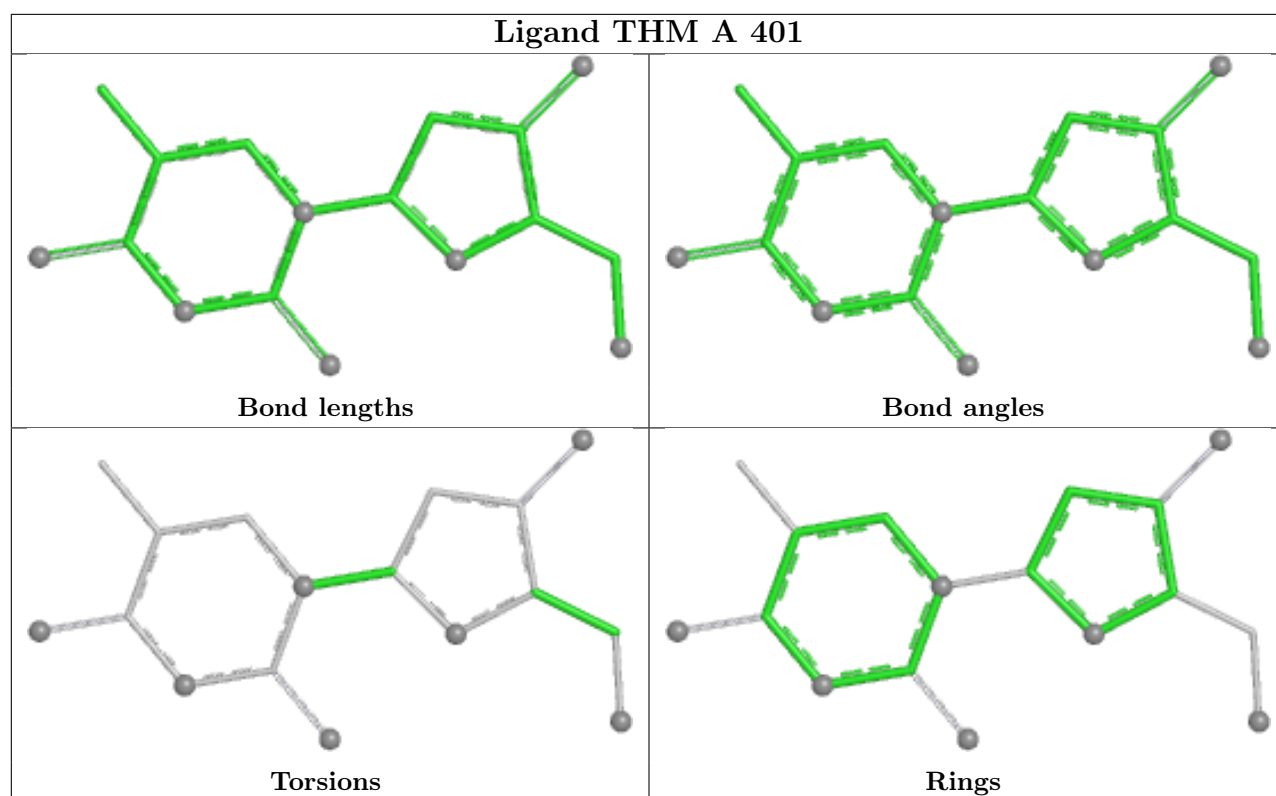
1 monomer is involved in 1 short contact:

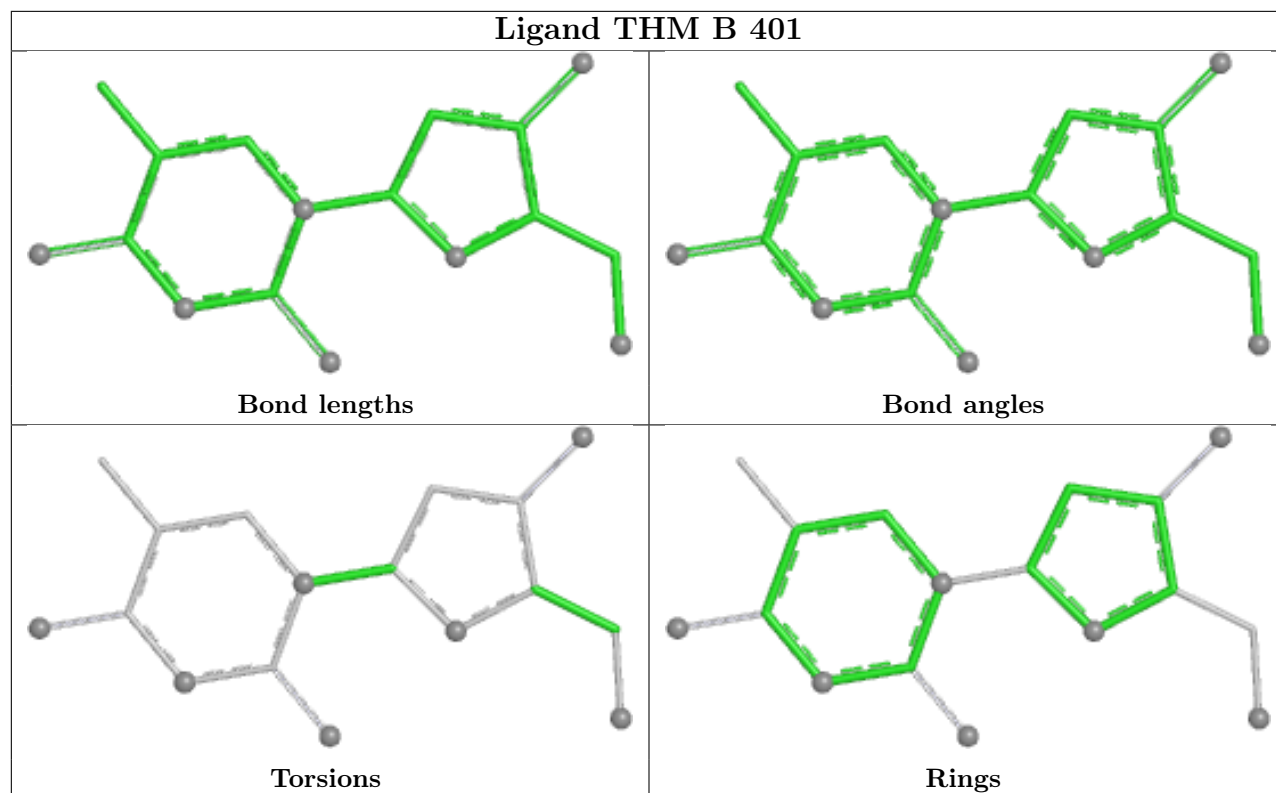
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	313/328 (95%)	0.37	12 (3%)	44	39	55, 76, 109, 180	0
1	B	313/328 (95%)	0.43	12 (3%)	44	39	52, 71, 102, 195	0
1	C	313/328 (95%)	0.61	21 (6%)	24	20	51, 83, 134, 209	0
1	D	313/328 (95%)	0.55	13 (4%)	40	36	55, 84, 121, 178	0
1	E	313/328 (95%)	0.60	19 (6%)	27	22	61, 91, 131, 177	0
1	F	313/328 (95%)	0.56	17 (5%)	31	27	58, 87, 120, 164	0
All	All	1878/1968 (95%)	0.52	94 (5%)	34	29	51, 83, 124, 209	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	46	LEU	5.0
1	B	293	ILE	4.9
1	F	287	PHE	4.8
1	E	305	ILE	4.7
1	F	306	ILE	4.6
1	C	35	VAL	4.4
1	A	321	PHE	4.4
1	E	317	PHE	4.3
1	E	284	MET	4.3
1	F	321	PHE	4.2
1	F	224	VAL	4.0
1	B	74	ILE	3.8
1	C	142	GLY	3.6
1	E	101	TYR	3.6
1	C	102	SER	3.6
1	C	305	ILE	3.5
1	C	82	ALA	3.4
1	F	305	ILE	3.4
1	E	290	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	105	PRO	3.4
1	E	63	LEU	3.3
1	E	105	PRO	3.3
1	C	304	GLU	3.3
1	A	289	LEU	3.2
1	E	293	ILE	3.2
1	C	321	PHE	3.1
1	B	253	SER	3.1
1	A	293	ILE	2.9
1	A	261	PHE	2.9
1	C	101	TYR	2.9
1	A	306	ILE	2.9
1	D	288	GLU	2.9
1	F	19	ASP	2.8
1	D	102	SER	2.8
1	D	105	PRO	2.8
1	F	320	GLU	2.8
1	F	293	ILE	2.7
1	D	63	LEU	2.7
1	D	82	ALA	2.7
1	E	168	ILE	2.7
1	F	74	ILE	2.7
1	B	294	ASP	2.7
1	D	23	ASP	2.6
1	B	101	TYR	2.6
1	B	244	VAL	2.5
1	D	305	ILE	2.5
1	B	211	VAL	2.5
1	B	26	SER	2.5
1	D	147	ILE	2.4
1	C	293	ILE	2.4
1	E	147	ILE	2.4
1	D	321	PHE	2.4
1	E	237	ILE	2.4
1	E	228	GLN	2.4
1	C	22	PHE	2.3
1	F	289	LEU	2.3
1	E	19	ASP	2.3
1	B	100	ILE	2.3
1	D	139	PHE	2.3
1	B	121	ALA	2.2
1	D	57	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	300	ILE	2.2
1	C	14	VAL	2.2
1	F	66	ALA	2.2
1	D	204	GLY	2.2
1	F	173	ILE	2.2
1	C	48	LEU	2.2
1	E	70	LEU	2.2
1	C	70	LEU	2.1
1	C	296	LEU	2.1
1	F	103	ASN	2.1
1	E	156	GLU	2.1
1	C	91	ASP	2.1
1	A	113	MET	2.1
1	E	122	PHE	2.1
1	F	121	ALA	2.1
1	E	123	LEU	2.1
1	A	119	GLU	2.1
1	C	9	SER	2.1
1	B	321	PHE	2.1
1	C	47	VAL	2.1
1	A	223	GLY	2.1
1	A	305	ILE	2.1
1	B	102	SER	2.1
1	C	90	PRO	2.1
1	A	35	VAL	2.0
1	F	244	VAL	2.0
1	F	285	ILE	2.0
1	F	282	PRO	2.0
1	E	17	ILE	2.0
1	E	252	THR	2.0
1	C	72	TRP	2.0
1	A	105	PRO	2.0
1	D	9	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

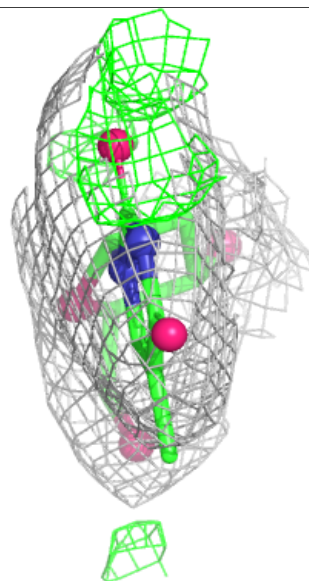
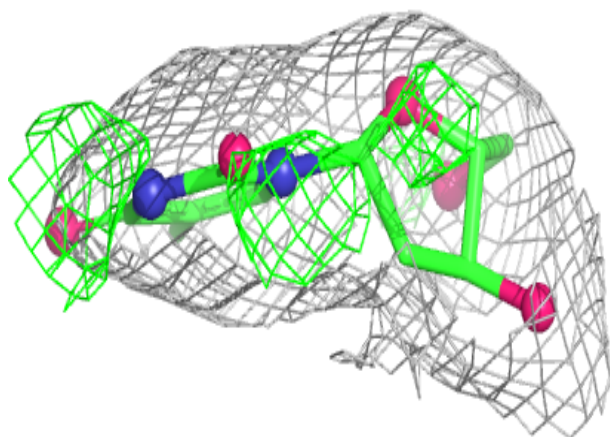
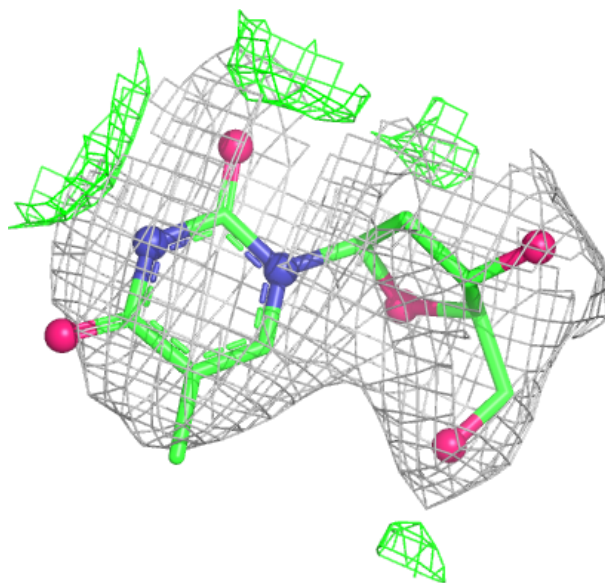
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	F	402	4/4	0.73	0.23	85,85,98,99	0
2	THM	E	401	17/17	0.89	0.11	59,77,83,85	0
2	THM	A	401	17/17	0.91	0.10	45,59,67,67	0
2	THM	F	401	17/17	0.92	0.11	62,69,90,91	0
2	THM	C	401	17/17	0.93	0.08	51,59,68,72	0
4	CL	D	402	1/1	0.94	0.10	82,82,82,82	0
4	CL	B	402	1/1	0.95	0.15	94,94,94,94	0
2	THM	B	401	17/17	0.95	0.10	50,56,68,71	0
2	THM	D	401	17/17	0.95	0.08	49,64,73,73	0
3	SO4	A	402	5/5	0.98	0.07	62,64,74,77	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

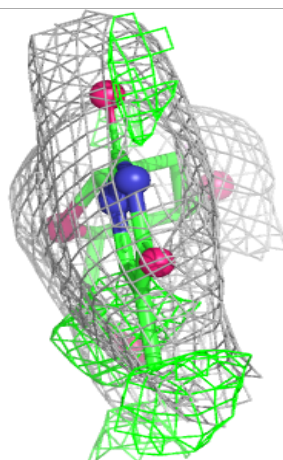
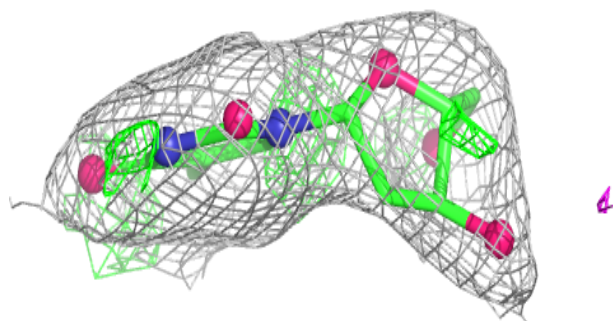
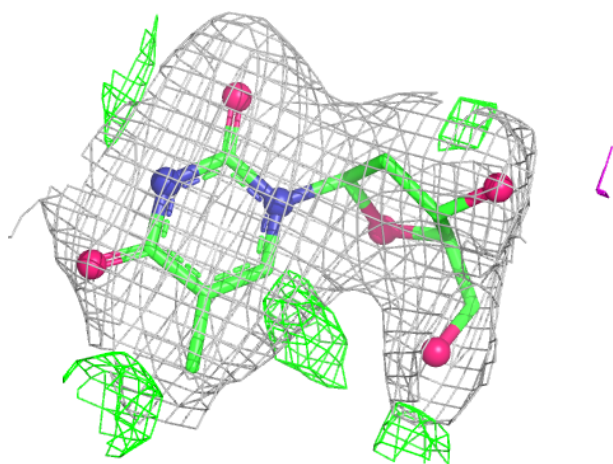
Electron density around THM E 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



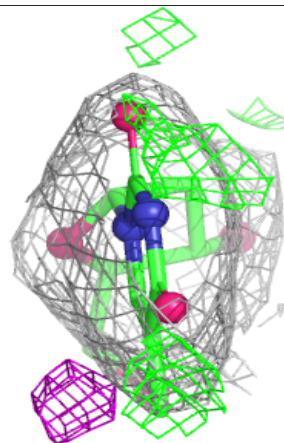
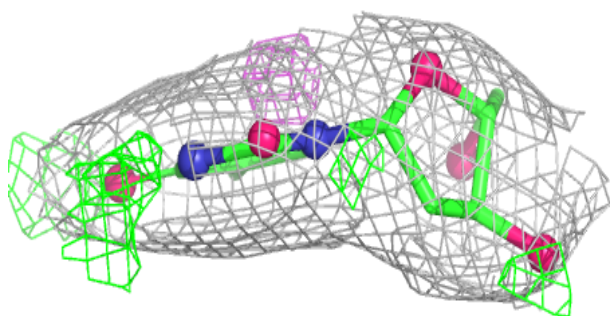
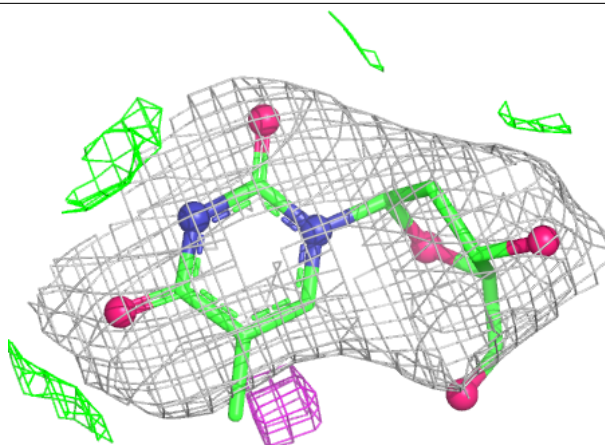
Electron density around THM A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



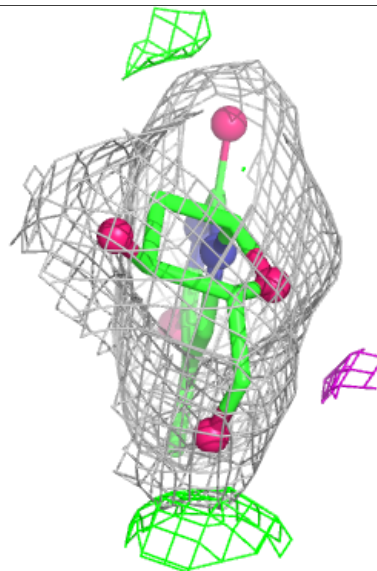
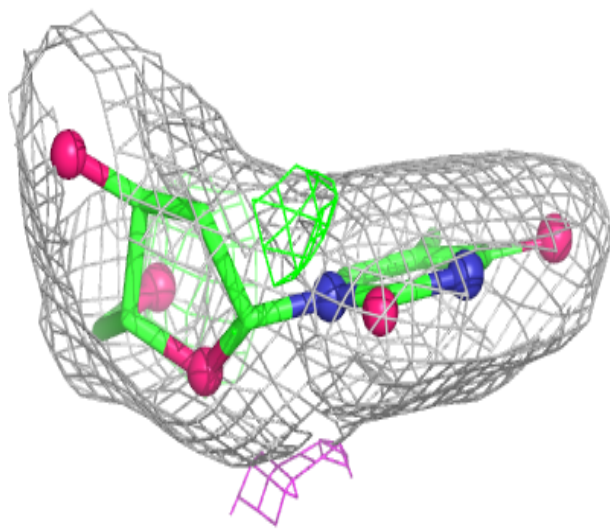
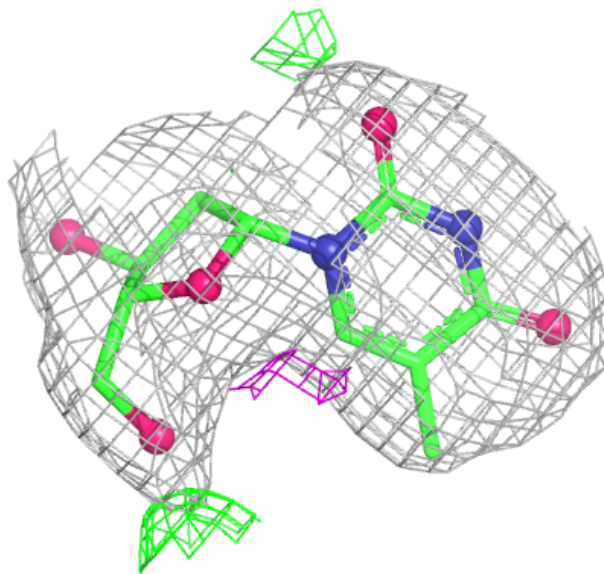
Electron density around THM F 401:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



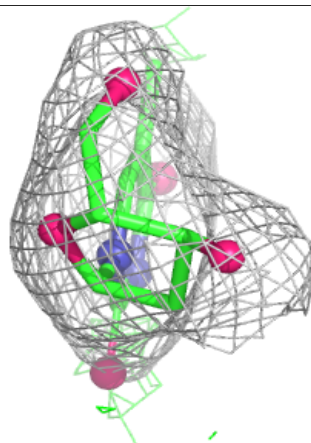
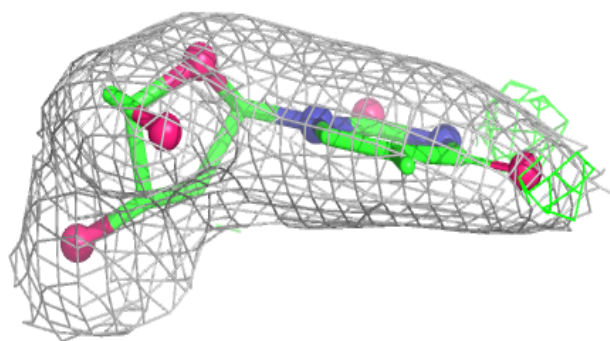
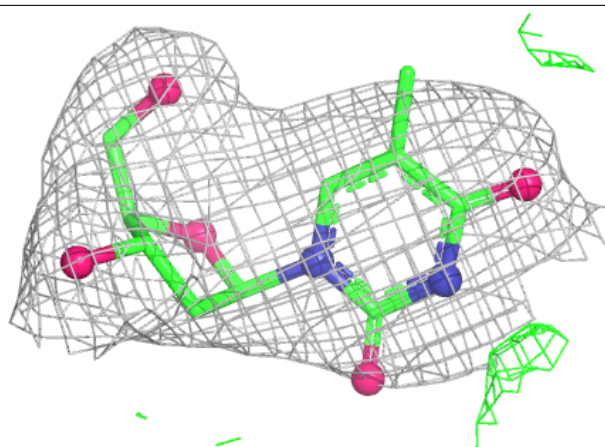
Electron density around THM C 401:

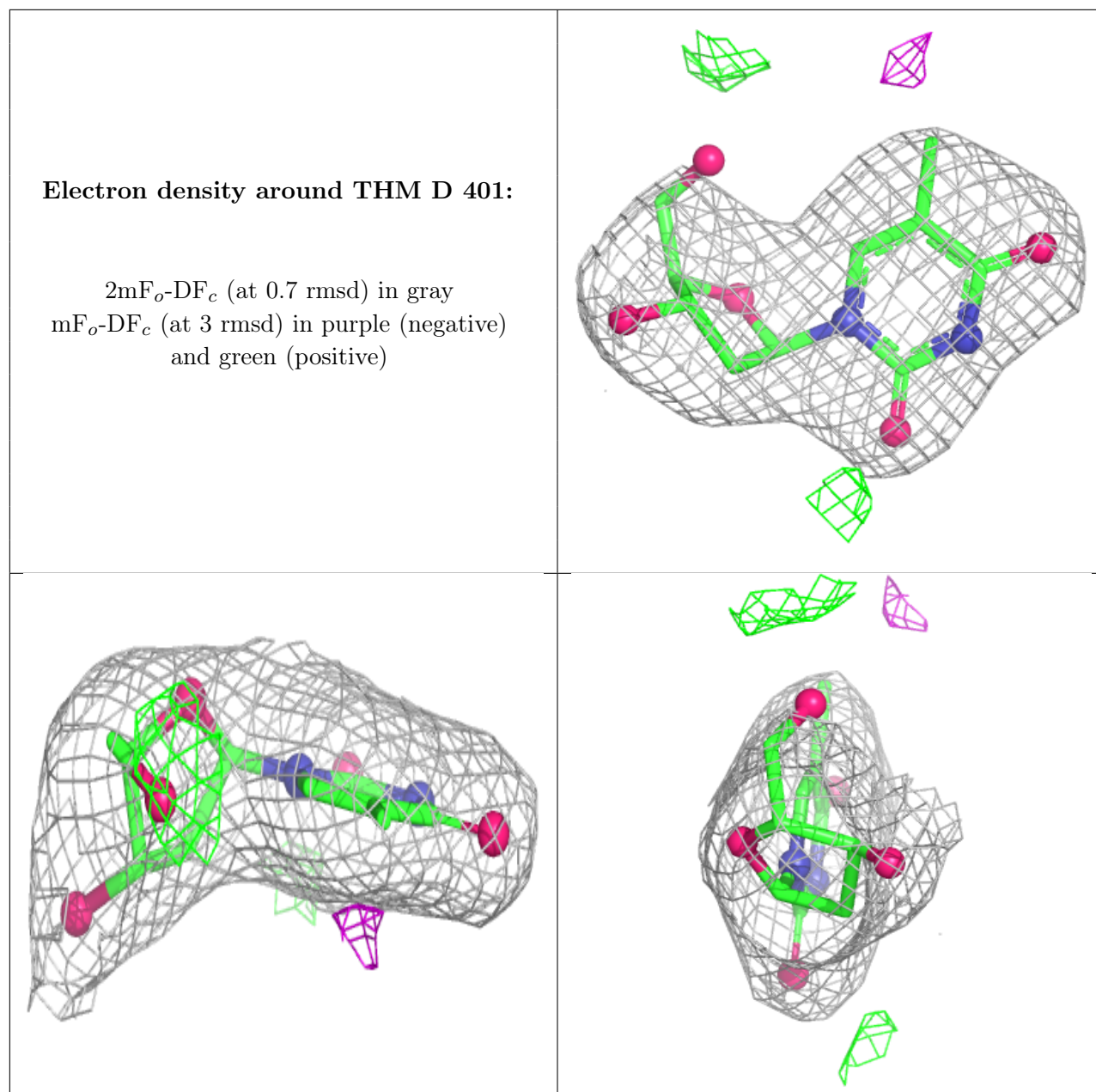
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around THM B 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.